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# **QUANTUM COMPUTING IN CONDENSED MATTER SYSTEMS**

**Clarkson University**

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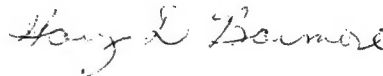
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## QUANTUM COMPUTING IN CONDENSED MATTER SYSTEMS

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# QUANTUM COMPUTING IN CONDENSED MATTER SYSTEMS

**Report Prepared by Dr. Vladimir Privman, Principal Investigator**

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## ABSTRACT

This project has accomplished all the scheduled tasks. Research program on feasibility of quantum computing in condensed matter systems has been initiated. Specific research results for several quantum logic gates, including the NOT gate, quantum signal splitting, and quantum copying, were obtained and prepared for publication. Directions for future work have been identified, including scope, impact, tools and collaborations needed. The first steps towards establishing a collaboration involving Air Force, Computer Science, and Physics investigators were taken.

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## 1.0 EXECUTIVE SUMMARY

This is a general summary and overview of results, ideas, background, and future plans. Specific details of the work accomplished, and literature references, are given in Sections 2.0, 3.0, 4.0.

### 1.1 What is Quantum Computing

In the seventies and eighties the size of computer components was decreasing nearly linearly and if the trend of then would continue, today's computer components would be zero size! However, in the nineties the relentless drive of industries and governments towards miniaturization of computer circuitry has slowed down. Most of the reasons for this have thus far been in manufacturing. Indeed, a recent Scientific American article (August 1996, p. 33) projects that the *next generation* of components (time scale 1-2 years) will be  $0.25\text{ }\mu\text{m}$  in dimensions. This size is  $2500\text{ }\text{\AA}$ , i.e., it is still well above the atomic dimensions.

It has become clear, however, that as the miniaturization continues, atomic dimensions will be reached, perhaps, with technology different from today's semiconductors. Then, quantum-mechanical effects will have to be considered in computer operation. A "passive" approach driven by this expectation has led some early workers to consider how quantum mechanics affects the foundations of computer science. Questions such as limitations on "classical" computation due to quantum fluctuations, quantum noise, etc., have been investigated.

A more "active" approach, initiated recently by several research groups which, in the USA, have been mainly based in industrial and government research labs (IBM, AT&T, Xerox, Los Alamos, etc.), is to attempt to harness the quantum nature of components of atomic dimensions for more efficient computation and design. This ambitious program involves many interesting scientific concepts new to both Computer Science and Physics communities. It also calls for new, nontraditional collaborations.

In order to answer whether quantum computation is feasible and useful, several issues must be addressed:

- Is quantum computation faster than classical computation?
- Can quantum computational elements be built and combined with other quantum and/or classical components?
- What will be the "design" rules for quantum computer components in order to perform Boolean logic operations?

- What are the error correction requirements and methods in quantum computation?

The answers to some of the questions that result from consideration of these general issues are still in the future. However, some definitive results have already been obtained. Specifically, on the theoretical side, new fast quantum algorithms have been proposed. One of these, due to Shor, allows fast factoring of numbers thus yielding an approach to break “unbreakable” cryptographic security codes. Error correction and unitary operations corresponding to the simplest logic gates have been explored in the literature. On the side of experiment, there are several atomic-scale systems where the simplest quantum-gate functions have been recently realized. There are also several promising condensed matter systems in which quantum-coherent processes can be maintained, usually controlled by laser radiation.

## 1.2 The Scope of the Present and Future Work

Our aim has been to investigate the feasibility of quantum computing in condensed matter systems. Condensed matter is the most promising medium for making small computational components. A collaboration involving theoretical physics, experimental materials science, and design-oriented computer engineering specialists is needed for long-term progress in this program; this has been organized and coordinated by Dr. Hotelling at the Rome Air Force Laboratory.

The effort at Clarkson University, by this PI, has been based on the following assumptions. We deem it inevitable that quantum properties of matter on the atomic scale will have to be considered in computer component design and use. However, it is still a long way to go, with modern technology, to a really “desktop” fully coherent quantum computational unit. *A more realistic expectation is that technological advances will soon allow design and manufacturing of limited-size units, based on several tens of atomic two-level systems, operating in a quantum-coherent fashion over a large time interval and possibly driven externally by laser beams.* These units will then become parts of a larger “classical” computer which will not maintain a quantum-coherent operation over its macroscopic dimensions.

Our program consists therefore of the following steps:

- Study the simplest quantum logic gates in order to identify which Hamiltonians are typical for interactions required for their operation. *In the present project we already made progress in this direction and obtained several specific results to be detailed in Sections 2.0, 3.0, 4.0.* In a longer run, we will need to collaborate with materials-science experimentalists to identify how these interactions can be realized in materials.



- Design systems of order 20 to 25 two-state atomic “components” with general-parameter interactions identified in the earlier step. Then, by using ordinary computers find those interaction value choices for which the resulting computational unit will be useful as part of a computer and will be usable for Boolean logic operations (this need of numerical calculations limits the number of constituents to 20-25, i.e., to systems with total of  $2^{20}$  to  $2^{25}$  states that modern computers can handle). In this stage, collaboration with computer design engineers will be crucial.
- Identification of how to incorporate such computational units in actual computer design. Here the emphasis shifts to Computer Science. Indeed, presently the approach in computer design is to build logical circuits from the simplest logic gates, such as NOT, AND, OR, NAND, etc. These usually involve one or two input bits and one output bit. Their operation is irreversible (dissipative). On the other hand, the quantum-computer components will involve several quantum-bits (qubits) as input and output. Their “built-in” Boolean function will be quite complicated. Furthermore, the rules of their interconnection with each other and with the rest of the “classical” computer will be different from today’s devices. Thus, a whole new branch of computer design engineering will have to emerge.

As stated earlier, we are presently in the initial stages of the first step in this program. Results achieved to date are outlined in Section 1.3 and detailed in Sections 2.0, 3.0, 4.0.

### **1.3 Tasks Accomplished within This Project**

The following specific research results have been obtained in this project.

- We studied the Hamiltonian for the quantum equivalent of the NOT computer gate. Explicit expression was obtained for the interaction parameters. Section 2.0 details this study, the results of which were submitted for publication in Physical Review A.
- Quantum signal splitting, of relevance to eavesdropping on transmission lines, has been investigated with emphasis on the way to accomplish a variant of signal splitting without limiting the initial quantum states of the systems in which the copies are recorded. Explicit interaction Hamiltonian was obtained. Section 3.0 provides the details of this study. The results were submitted for publication in Physical Review Letters.
- Quantum copying, important in error-correction protocols, has been investigated with the aim of deriving an explicit Hamiltonian for this process. The results are being presently prepared for publication. Section 4.0 details this study.

In addition to the specific research projects, we have established long-term collaboration with Dr. Hotaling of the Rome Laboratory, with Prof. Pease of Syracuse University, and developed contacts with several other researchers in the field. A "vision for the future" to define the follow-up research directions has been established and presented in the Section 1.2. A graduate student has been identified who is qualified to work within the planned research effort.

#### 1.4 Publications

The following publications have been written presenting the results of this project:

*Design of gates for quantum computation: the NOT gate*, D. Mozyrsky, V. Privman and S.P. Hotaling, submitted to Physical Review A.

*Quantum signal splitting as entanglement due to three-spin interactions*, D. Mozyrsky and V. Privman, submitted to Physical Review Letters.

*A Hamiltonian for Quantum Copying*, D. Mozyrsky, V. Privman and M. Hillery, in preparation, to be submitted to Physics Letters A.

#### 1.5 Presentations and Educational Impact

The following presentations have resulted from this project:

D. Mozyrsky (a graduate student) gave an informal talk on quantum computing to Physics faculty and students at Clarkson University on September 13, 1996.

S.P. Hotaling gave a Physics colloquium at Clarkson University on September 20, 1996 entitled *Introductory Comments on Quantum Computing*.

V. Privman gave a Condensed Matter seminar at SUNY Buffalo on September 27, 1996 entitled *Hamiltonians for Quantum Computing*.

Abstracts will be submitted for 3 presentations at the SPIE conference next Spring.

The above seminar presentations were attended largely by graduate students, and some undergraduates. One of the coauthors of the papers listed in Section 1.4, Mr. Mozyrsky, is a graduate student at Clarkson University. Thus, the educational impact of this project has been mainly at the level of graduate student training and exposure to the subject of quantum computing.

## 2.0 THE QUANTUM NOT GATE

We studied interactions needed to operate the quantum-mechanical NOT gate in the conventional formulation when the evolution is in time only and also in the case of *spatially separated Input and Output* two-state systems. Explicit expressions for the Hamiltonian were derived for the interaction which is time-independent for the duration of the gate operation. We developed a general approach which can be used to obtain Hamiltonians of this sort for quantum computer gates. We also discussed extensions to the case of time-dependent interactions. (This section is self-contained.)

### 2.1 Introduction

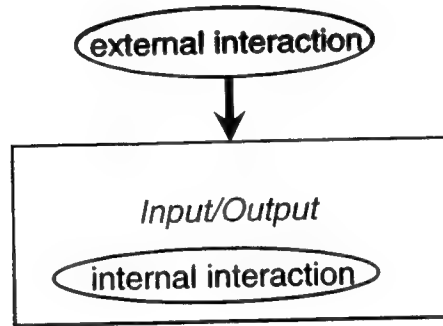
Quantum mechanics of computation is a rather active field of study; we provide a partial list of a review-type literature [2.1-2.26]. The ultimate goal would be to construct a macroscopic quantum system which would function as a programmable calculational apparatus. However, this goal is elusive [2.16,2.18]. Nevertheless, with the relentless drive towards miniaturization of computer components, quantum-mechanical behavior will have to be considered [2.14-2.16,2.18] seriously in their design. Experimental advances have recently been reported [2.25,2.27-2.28] yielding the first functional examples of “quantum gates” which can be controlled without losing quantum coherence. Quantum computing also has tremendous “basic science” value in offering new challenges and experimental connections in the field of theoretical foundations of quantum mechanics, in understanding the decoherence effects on quantum evolution, e.g., [2.16,2.18,2.26,2.29-2.31], and in derivation of inherently quantum-mechanical computational algorithms, e.g., [2.29-2.30,2.32-2.35].

A typical “classical” computer gate, for instance, in a solid-state device, is structured as shown in Figure 1. The *Input* signal is converted into the *Output* signal by interactions in the connecting “circuitry.” There is an internal time scale,  $\Delta t$ , for the gate operation. It is determined by the dynamics of the circuitry which includes the *dissipation processes* in it. Such a gate is therefore irreversible dynamically even though it might perform a reversible logical operation such as the NOT function. In fact, it has been established that *any* logical operation sequence can be accomplished reversibly in the “logics” sense; see, e.g., [2.36]. However, the dynamical evolution of the underlying solid-state device need not be reversible; see, e.g., [2.18,2.26] for general discussion.

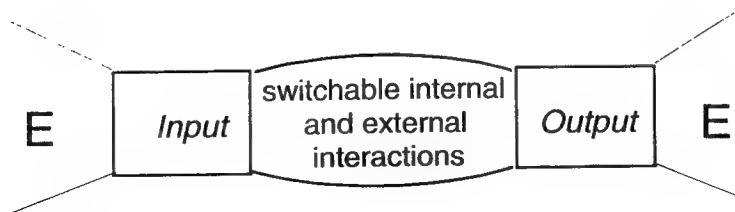
In quantum computation, the “logics” ingredient is supposed to go beyond the “classical” case by using the *quantum interference*, i.e., by exploiting the fact that a quantum-mechanical system can be in a superposition of basic states, such as the *up* and *down* states of a bit, termed in this context a “qubit.” Therefore ideally any source



**Figure 1:** The “classical” computer gate.



**Figure 2:** Quantum gate operation by evolution in time. The *Input* and *Output* are both states of the same system.



**Figure 3:** Quantum gate with spatially separated *Input* and *Output*. Interactions with components of the system which are external to this gate are schematically marked by *E*.

of decoherence, such as dissipation processes and other uncontrolled interactions with the environment must be avoided. It is presently not clear how far can the modern technology go in this direction [2.16,2.18] and how much of the decoherence can be repaired by various “error correction” schemes, e.g., [2.26,2.29-2.31].

Thus, both the quantum logics and the dynamics of the gate should ideally be fully reversible. Implications of this property have biased recent literature on the quantum logic gates. Firstly, the distinction between the *Input* part and the *Output* part of the system has been blurred. A typical configuration is that of Figure 2. The same quantum-mechanical system is “programmed” with the *Input* and then after the time interval  $\Delta t$  it will be in the *Output* state. We note that the time interval  $\Delta t$  is fully determined by the parameters of the Hamiltonian. Alternatively, we can conclude that in order to effect the quantum gate operation, the interaction energies associated with both the internal and external-field parts of the Hamiltonian must be of order  $\hbar/\Delta t$ .

Secondly, consideration of the full quantum system requires a large number of basis states. As a result, there are virtually no explicit examples available of what the actual interaction Hamiltonians should look like in simple quantum gates. One notable exception is the NOT gate operation in a two-state system [2.10] obtained by applying an external magnetic field on a single spin. Then another field is applied, oscillating in time, in a direction perpendicular to the constant field component. This “paramagnetic resonance” problem is well known solvable “textbook” example of time-dependent quantum-mechanical evolution.

Another approach has been to consider interactions switched on only for the duration of the gate operation  $\Delta t$ . If the “gate” is actually the whole computer then one can regard the interaction as time-independent. However, for specific operations in components with a limited number of basis states, it may be appropriate to view the interaction as controlled externally to be switched on and off. While general ideas of externally timed computation are not new, see [2.18] for a discussion, actual realizations of such a system in quantum computation may be as technologically challenging as maintaining coherence, etc. General developments for the latter type of interaction (time-independent or on/off) have included identification of unitary operators that correspond to quantum computer operation and establishment of the existence of the appropriate interaction Hamiltonians [2.5,2.21].

A useful view of a computer component can be obtained by trying to generalize the configuration of Figure 1 to the quantum case. This is shown in Figure 3; what we have in mind is a part of the computer that performs a single operation whereby the *Input* state determines the *Output* state after a time interval  $\Delta t$ . The interactions

must be controlled, i.e., switched on and off, in order for us to be able to consider the gate operation during the interval  $\Delta t$  independent of the interactions with the computer parts external (marked E in the figure) to the gate. This control of interaction, i.e., external timing of the computer operation already mentioned earlier, can be possibly accomplished by the external interactions while the internal interactions be reserved for the gate operation. One of our objectives will be to check this expectation.

The goal of this part of the project is to develop expressions for possible interaction Hamiltonians and identify techniques useful in general derivations of this sort. Our actual calculations will be for the NOT gate. In Section 2.2, we consider the simplest NOT gate of the type described in Figure 2, i.e., a two-state system where the NOT operation is accomplished by an external interaction. This system has already been studied extensively in the literature, e.g., [2.1,2.3,2.9-2.11,2.21]. However, we believe that our main result, equation (12) below, for the interaction Hamiltonian is new. The calculations are simple and they are used to set up our notation and exemplify some general principles.

A more complicated, and in our opinion more interesting, NOT gate, viewed as a computer component, with spatially separated *Input* and *Output*, see Figure 3, is studied in Section 2.3. Our main result, equation (21) below, establishes that such a NOT gate can be operated by the internal interactions alone so that external-field effects can be reserved for the clocking of the internal interactions. Furthermore, it suggests the type of local internal interactions to be used in more complicated systems where the computer as a whole is treated as a many-body system with time-independent interactions.

Regarding the requirement to control the interactions externally, with the time dependence given by the on/off “protocol,” in Section 2.4 we extend our approach to certain other time-dependent interactions (protocols) which are more smooth than the on/off shape. Section 2.4 also offers a summarizing discussion.

## 2.2 The Single-Qubit NOT Gate

In this section we consider the NOT gate based on a two-state system. Such a gate has been extensively studied in the literature, e.g., [2.1,2.3,2.9-2.11,2.21], so that part of our discussion is a review intended to set up the notation and illustrate methods useful in more complicated situations. We label by  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$  the two basis states. The NOT gate corresponds to those interactions which, over the time interval  $\Delta t$ , accomplish the following changes:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow e^{i\alpha} \begin{pmatrix} 0 \\ 1 \end{pmatrix} , \quad (1)$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \Rightarrow e^{i\beta} \begin{pmatrix} 1 \\ 0 \end{pmatrix} . \quad (2)$$

The phases  $\alpha$  and  $\beta$  are arbitrary. The unitary matrix  $U$ , that corresponds to this evolution, is uniquely determined,

$$U = \begin{pmatrix} 0 & e^{i\beta} \\ e^{i\alpha} & 0 \end{pmatrix} . \quad (3)$$

The eigenvalues of  $U$  are given by

$$u_1 = e^{i(\alpha+\beta)/2} \quad \text{and} \quad u_2 = -e^{i(\alpha+\beta)/2} , \quad (4)$$

while the (right) eigenvectors, when normalized and regarded as matrix columns, yield the following (unitary) transformation matrix  $T$  which can be used to diagonalize  $U$ :

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta/2} & e^{i\beta/2} \\ e^{i\alpha/2} & -e^{i\alpha/2} \end{pmatrix} . \quad (5)$$

Thus, we have

$$T^\dagger U T = \begin{pmatrix} u_1 & 0 \\ 0 & u_2 \end{pmatrix} . \quad (6)$$

Here the dagger superscript denotes Hermitian conjugation.

We next use the general relation

$$U = e^{-iH\Delta t/\hbar} \quad (7)$$

to identify the (time-independent) Hamiltonian in the diagonal representation. Relations (4) yield the energy levels:

$$E_1 = -\frac{\hbar}{2\Delta t}(\alpha + \beta) + \frac{2\pi\hbar}{\Delta t}N_1, \quad E_2 = -\frac{\hbar}{2\Delta t}(\alpha + \beta) + \frac{2\pi\hbar}{\Delta t}\left(N_2 + \frac{1}{2}\right), \quad (8)$$

where  $N_1$  and  $N_2$  are arbitrary integers. The Hamiltonian is then obtained from the relation

$$H = T \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} T^\dagger \quad (9)$$

as a certain  $2 \times 2$  matrix. The latter is conveniently represented in terms of the unit matrix  $\mathcal{I}$  and the conventional Pauli matrices  $\sigma_x$ ,  $\sigma_y$ ,  $\sigma_z$ . We get

$$H = \left[ -\frac{\hbar}{2\Delta t}(\alpha + \beta) + \frac{\pi\hbar}{\Delta t} \left( N_1 + N_2 + \frac{1}{2} \right) \right] \mathcal{I} \\ + \frac{\pi\hbar}{\Delta t} \left( N_1 - N_2 - \frac{1}{2} \right) \left[ \left( \cos \frac{\alpha - \beta}{2} \right) \sigma_x + \left( \sin \frac{\alpha - \beta}{2} \right) \sigma_y \right] . \quad (10)$$

To effect the gate operation, the interaction must be switched on for the time interval  $\Delta t$ . The constant part of the interaction energy (the part proportional to the unit matrix  $\mathcal{I}$ ) is essentially arbitrary; it only affects the average phase  $\frac{\alpha + \beta}{2}$  of the transformation (1)-(2). Thus this term can be disregarded.

The nontrivial part of (10) depends on the integer  $N = N_1 - N_2$  which is arbitrary, and on one arbitrary angular variable

$$\gamma = \frac{\alpha - \beta}{2} . \quad (11)$$

Thus we can use the Hamiltonian in the form

$$H = \frac{\pi\hbar}{\Delta t} \left( N - \frac{1}{2} \right) [(\cos \gamma) \sigma_x + (\sin \gamma) \sigma_y] . \quad (12)$$

For a spin- $\frac{1}{2}$  two-state system such an interaction can be obtained by applying a magnetic field oriented in the  $XY$ -plane at an angle  $\gamma$  with the  $X$ -axis. The strength of the field is inversely proportional to the desired time interval  $\Delta t$ , and various allowed field values are determined by the choice of  $N$ .

We note that during application of the external field the *up* and *down* quantum states in (1)-(2) are *not* the eigenstates of the Hamiltonian. If the time interval  $\Delta t$  is not short enough, the energy-level splitting  $|E_1 - E_2| \propto |N - \frac{1}{2}|$  can result in spontaneous emission which is just one of the undesirable “noise” effects destroying quantum



coherence. Generally, when implemented in a condensed matter matrix for instance, the two states of the qubit may lie within a spectrum of various other energy levels. In that case, in order to minimize the number of spontaneous transition modes, the best choice of the interaction strength would correspond to minimizing  $|E_1 - E_2|$ , i.e., to  $|N - \frac{1}{2}| = \frac{1}{2}$ .

### 2.3 The Spatially Extended NOT Gate

In this section we consider the spatially extended NOT gate shown in Figure 3. We will describe the two two-state systems (*Input* and *Output*) by four-state vectors and matrices labeled according to the following self-explanatory convention:

$$\begin{aligned} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} &= a_1 |\uparrow\uparrow\rangle + a_2 |\uparrow\downarrow\rangle + a_3 |\downarrow\uparrow\rangle + a_4 |\downarrow\downarrow\rangle \\ &= a_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_I \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_O + a_2 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_I \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_O \\ &\quad + a_3 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_I \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_O + a_4 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_I \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_O . \end{aligned} \tag{13}$$

Here  $I$  and  $O$  denote *Input* and *Output*. In what follows we will omit the direct-product symbols  $\otimes$  when multiplying expressions with subscripts  $I$  and  $O$ .

The desired transformation should take any state with  $a_3 = a_4 = 0$  into a state with components 1 and 3 equal zero, i.e., *Input up* yields *Output down*. Similarly, any state with  $a_1 = a_2 = 0$  should evolve into a state with components 2 and 4 equal zero, corresponding to *Input down* giving *Output up*. The general evolution operator must therefore be of the form

$$U = \begin{pmatrix} 0 & 0 & U_{13} & U_{14} \\ U_{21} & U_{22} & 0 & 0 \\ 0 & 0 & U_{33} & U_{34} \\ U_{41} & U_{42} & 0 & 0 \end{pmatrix} , \tag{14}$$

which depends on 16 real parameters. However, one can show that the requirement of unitarity,  $U^\dagger U = 1$ , imposes 8 conditions so that the number of real parameters is reduced to 8. A lengthy but straightforward algebraic calculation then shows that the following parametrization covers all such unitary matrices:

$$U = \begin{pmatrix} 0 & 0 & e^{i\chi} \sin \Omega & e^{i\beta} \cos \Omega \\ -e^{i(\alpha+\rho-\eta)} \sin \Upsilon & e^{i\rho} \cos \Upsilon & 0 & 0 \\ 0 & 0 & e^{i\delta} \cos \Omega & -e^{i(\beta+\delta-\chi)} \sin \Omega \\ e^{i\alpha} \cos \Upsilon & e^{i\eta} \sin \Upsilon & 0 & 0 \end{pmatrix}. \quad (15)$$

Here all the angular variables are unrestricted although we could limit  $\Omega$  and  $\Upsilon$  to the range  $[0, \frac{\pi}{2}]$  without loss of generality.

In order to make the calculation analytically tractable, we will restrict the number of free parameters to four by considering the case

$$U = \begin{pmatrix} 0 & 0 & 0 & e^{i\beta} \\ 0 & e^{i\rho} & 0 & 0 \\ 0 & 0 & e^{i\delta} & 0 \\ e^{i\alpha} & 0 & 0 & 0 \end{pmatrix}. \quad (16)$$

This form has been favored for the following reasons. Firstly, the structure of a single phase-factor in each column is similar to that of the two-dimensional matrix encountered in Section 2.2. Secondly, the form (16) contains Hermitian-U cases ( $\beta = -\alpha$ ,  $\rho = 0$  or  $\pi$ ,  $\delta = 0$  or  $\pi$ ). Therefore, the eigenvalues, which are generally on the unit circle for any unitary matrix, may be positioned more symmetrically with respect to the real axis, as functions of the parameters. These observations suggest that an analytical calculation may be possible.

Indeed, the eigenvalues of  $U$  turn out to be quite simple:

$$u_1 = e^{i(\alpha+\beta)/2}, \quad u_2 = -e^{i(\alpha+\beta)/2}, \quad u_3 = e^{i\rho}, \quad u_4 = e^{i\delta}. \quad (17)$$

The (unitary) diagonalizing matrix  $T$  made up of the normalized (right) eigenvectors as columns is

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta/2} & e^{i\beta/2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} \\ e^{i\alpha/2} & -e^{i\alpha/2} & 0 & 0 \end{pmatrix}. \quad (18)$$

The next step in the calculation is to identify the energy levels. We chose the notation such that the energies  $E_{1,2}$  are identical to (8). The other two energies are given by

$$E_3 = -\frac{\hbar}{\Delta t}\rho + \frac{2\pi\hbar}{\Delta t}N_3, \quad E_4 = -\frac{\hbar}{\Delta t}\delta + \frac{2\pi\hbar}{\Delta t}N_4, \quad (19)$$

The Hamiltonian is then obtained as in Section 2.2. It is convenient to avoid cumbersome expressions by expressing it in terms of the energies; the latter will be replaced by explicit expressions (8), (19) when needed. The resulting  $4 \times 4$  matrix has been expressed in terms of the direct products involving the unit matrices and the Pauli matrices of the *Input* and *Output* two-state systems. This calculation is straightforward but rather lengthy. We only report the result:

$$\begin{aligned} H = & \frac{1}{4}(2E_1 + 2E_2 + E_3 + E_4) + \frac{1}{4}(E_3 - E_4)(\sigma_{zI} - \sigma_{zO}) \\ & + \frac{1}{4}(2E_1 + 2E_2 - E_3 - E_4)\sigma_{zI}\sigma_{zO} \\ & + \frac{1}{4}(E_1 - E_2)\left(\cos\frac{\alpha - \beta}{2}\right)(\sigma_{xI}\sigma_{xO} - \sigma_{yI}\sigma_{yO}) \\ & + \frac{1}{4}(E_1 - E_2)\left(\sin\frac{\alpha - \beta}{2}\right)(\sigma_{xI}\sigma_{yO} + \sigma_{yI}\sigma_{xO}) . \end{aligned} \quad (20)$$

As in Section 2.2, we note that the constant part of the Hamiltonian can be changed independently of the other coupling constants and it can be discarded. Recall that we can generally vary the integers  $N_{1,2,3,4}$  and the variables  $\alpha, \beta, \rho, \delta$ . The “constant” part is in fact proportional to  $\mathcal{I}_I \otimes \mathcal{I}_O$ . However, we avoid this cumbersome notation and present the terms in the Hamiltonian in a more physically transparent form.

The Hamiltonian in (20) has also terms linear in the Pauli matrices (in the spin components for spin systems). These correspond to interactions with externally applied fields which in fact must be of opposite direction for the *Input* and *Output* spins. As explained in the introduction, we try to avoid such interactions: hopefully, external fields will only be used for “clocking” of the computation, i.e., for controlling the internal interactions via some intermediary part of the system connecting the *Input* and *Output* two-state systems; see Figure 3. Thus, we will assume that  $E_3 = E_4$  so that there are no terms linear in the spin components, in the Hamiltonian.

Among the remaining interaction terms, the term involving the  $z$ -components in the product form  $\sigma_{zI}\sigma_{zO}$  ( $\equiv \sigma_{zI} \otimes \sigma_{zO}$ ), has an arbitrary coefficient, say,  $-\mathcal{E}$ . The

terms of order two in the  $x$  and  $y$  components have free parameters similar to those in (11)-(12) in Section 2.2. The final expression is

$$H = -\mathcal{E}\sigma_{zI}\sigma_{zO} + \frac{\pi\hbar}{2\Delta t} \left( N - \frac{1}{2} \right) \left[ (\cos \gamma) (\sigma_{xI}\sigma_{xO} - \sigma_{yI}\sigma_{yO}) + (\sin \gamma) (\sigma_{xI}\sigma_{yO} + \sigma_{yI}\sigma_{xO}) \right] . \quad (21)$$

Here  $N = N_1 - N_2$  must be integer. In order to minimize the spread of the energies  $E_1$  and  $E_2$  we could choose  $|N - \frac{1}{2}| = \frac{1}{2}$  as in Section 2.2. Recall that we already have  $E_3 = E_4$ . Actually, the energy levels of the Hamiltonian in the notation (21) are

$$E_1 = -\mathcal{E} + \frac{\pi\hbar}{\Delta t} \left( N - \frac{1}{2} \right) , \quad E_2 = -\mathcal{E} - \frac{\pi\hbar}{\Delta t} \left( N - \frac{1}{2} \right) , \quad E_{3,4} = \mathcal{E} . \quad (22)$$

Thus further degeneracy (of three levels but not all four) can be achieved by varying the parameters.

## 2.4 Time-Dependent Interactions. Discussion

The form of the interactions in (21) is quite unusual as compared to the traditional spin-spin interactions in condensed matter models. The latter usually are based on the uniaxial (Ising) interaction proportional to  $\sigma_z\sigma_z$ , or the planar  $XY$ -model interaction proportional to  $\sigma_x\sigma_x + \sigma_y\sigma_y$ , or the isotropic (scalar-product) Heisenberg interaction. The spin components here are those of two different spins (not marked). The interaction (21) involves an unusually high degree of anisotropy in the system. The  $x$  and  $y$  components are coupled in a tensor form which presumably will have to be realized in a medium with well-defined directionality, possibly, a crystal.

All the interaction Hamiltonians considered thus far were constant for the duration of the gate operation. They must be externally controlled. However, we note that the application of the interaction need not be limited to the time-dependence which is an abrupt on/off switching. Indeed, we can modify the time dependence according to

$$H(t) = f(t)H , \quad (23)$$

where we use the same symbol  $H$  for both the original time-independent interaction Hamiltonian such as (21) and the new, time-dependent one,  $H(t)$ . The latter involves the “protocol” function  $f(t)$ . The shape of this function, nonzero during the operation of the gate from time  $t$  to time  $t + \Delta t$ , can be smooth.

For Hamiltonians involving externally applied fields, such as (12), it may be important to have a constant plus an oscillatory components (corresponding to constant and electromagnetic-wave magnetic fields, for instance). However, the protocol function must satisfy

$$\int_t^{t+\Delta t} f(t') dt' = \Delta t , \quad (24)$$

and therefore it cannot be purely oscillatory; it must have a constant or other contribution to integrate to a nonzero value in accordance with (24).

The possibility of the modification (23) follows from the fact that the general relation

$$U = \left[ e^{-i \int_t^{t+\Delta t} H(t') dt' / \hbar} \right]_{\text{time-ordered}} \quad (25)$$

does not actually require time ordering as long as the Hamiltonian commutes with itself at different times. This condition is satisfied by (23). Furthermore, if the Hamiltonian can be written as a sum of commuting terms then each term can be multiplied by its own protocol function. Interestingly, the Hamiltonian of the “paramagnetic resonance” NOT gate [2.10] mentioned in the Introduction, is not of this form. It contains a constant part and an oscillatory part but they do not commute. Note that the term proportional to  $\mathcal{E}$  in (21) commutes with the rest of that Hamiltonian. The terms proportional to  $\cos \gamma$  and  $\sin \gamma$  do not commute with each other though. Rather, they anticommute, in (21), as such terms do in (12).

In summary, we have derived expressions for the interaction Hamiltonians appropriate for the NOT gate operation in two-state systems. The expressions obtained will be useful in identifying materials where there is hope of actually realizing such gates, in writing down model Hamiltonians for more complicated, multi-gate configurations, and in studying these gates as individual components, for instance, with dissipation added.

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### 3.0 QUANTUM SIGNAL SPLITTING

The classical signal splitting and copying are not possible in quantum mechanics. Specifically, one cannot copy the basis up and down states of the input ( $I$ ) two-state system into the copy ( $C$ ) and duplicate-copy ( $D$ ) two-state systems if the latter systems are initially in an arbitrary state. We consider instead a quantum evolution in which the basis states of  $I$  at time  $t$  are duplicated in *at least two* of the systems  $I$ ,  $C$ ,  $D$ , at time  $t + \Delta t$ . For possible applications in quantum computing, we derive an explicit Hamiltonian to accomplish this process; it turns out to involve only three-spin  $x, y$ -component interactions. (This section is self-contained.)

#### 3.1 Introduction

Recent interest in quantum computing [3.1-3.27] has led to consideration of quantum dynamical processes mimicing computer gate operation, i.e., those processes that involve “binary” states constructed from the up and down states of two-state systems (qubits). The goal of making coherent quantum computational units is elusive [3.16,3.18]. However, miniaturization of computer components suggests that quantum-mechanical effects will have to be considered eventually [3.14-3.16,3.18] in their design. Experiments have recently been reported [3.25,3.28-3.29] realizing the simplest “quantum gates” which can be controlled without losing quantum coherence. Understanding the decoherence effects, e.g., [3.16,3.18,3.26,3.30-3.32], and derivation of inherently quantum-mechanical computational algorithms, e.g., [3.30-3.31,3.33-3.36], are of great “basic science” value.

The “classical” signal-copying process starts from the input value  $I$  and after some time  $\Delta t$  results in the same value at the copy  $C$  and, if needed, duplicate-copy  $D$ . We assume that the value of  $I$  is unchanged. This is the case when a signal is copied, for instance, by connecting wires and forcing the voltage in one of them to the value 0 or 1. This input-wire voltage, and the equilibrium state, will be established in all the connected wires, after a time  $\Delta t$  determined by the speed of light and relaxation time of the charge-carrier distribution in the wires. The important point to note is that this “classical” copying/duplicating of a signal is not governed by reversible dynamics; there are inevitably some irreversible dissipation processes involved.

Quantum-mechanical copying from  $I$  to  $C$ , for instance, has been discussed in the literature [3.37-3.40], as were more complicated, multi-copy processes. Generally, one cannot copy an arbitrary quantum state. However, one can duplicate a set of basis states of  $I$ , for instance, the qubit states up and down ( $|1\rangle$  and  $|0\rangle$ ). One can also discuss an approximate, optimized copying of the linear combinations of the basis states of  $I$



[3.39,3.40]. A major limitation of these copying procedures has been that the *initial* state of  $C$  (or more generally, of the systems which are imprinted with the copies) must be *fixed*. This feature makes it unlikely that any interesting interference effects will be involved in the process.

Here we explore those quantum-mechanical processes that retain some of the “classical” copying features but do not involve any restriction on the initial state of the system  $C$ , even though the property of making copies will be meaningful only for the basis states of the input system  $I$ .

If we require that the basis states of  $I$  at time  $t$  be copied in such a way that both  $I$  and  $C$ , and if needed, another copy  $D$ , are all in that basis state at time  $t + \Delta t$  for an arbitrary initial state of  $C$  (and  $D$ ), then one can easily verify that no unitary transformation can accomplish the desired mapping. Such quantum copying is not possible.

Our approach is to consider instead the process in which an initial state of  $I$ , from the basis set  $|1\rangle, |0\rangle$ , is duplicated in *at least two* of the three final states  $I, C, D$ . Thus, we consider three two-state systems. The initial state of  $I$ , as long as it is one of the qubit states, will be “multiplied” in such a way that at time  $t + \Delta t$  two or three of the systems  $I, C, D$ , are in that state, but we do not know if it is two or three, and in the case of two, which two are in that state. A unitary quantum evolution is possible that satisfies these conditions; we provide an explicit example.

### 3.2 A Quantum Signal-Splitting Hamiltonian

Let us label the states of the combined system  $I+C+D$  by  $|111\rangle, |110\rangle, |101\rangle, |100\rangle, |011\rangle, |010\rangle, |001\rangle, |000\rangle$ , where the order of the systems is  $|ICD\rangle$ . One can then check that unitary  $8 \times 8$  matrices can be found that accomplish the desired transformation. In fact, the requirement is that any linear combination of the states  $|1CD\rangle$  is mapped onto a linear combination of  $|111\rangle, |110\rangle, |101\rangle$  and  $|011\rangle$ , while any linear combination of the states  $|0CD\rangle$  is mapped onto a linear combination of  $|100\rangle, |010\rangle, |001\rangle$  and  $|000\rangle$ . The general unitary transformation actually has many free parameters; it is by no means limited or special. Many different quantum evolutions accomplish the task.

For our explicit calculations we choose the simplest root to the desired copying: we consider a unitary transformation that flips (and possibly changes phases of) the basis states only in the subspace of  $|100\rangle, |011\rangle$ . The  $8 \times 8$  unitary evolution matrix  $U$  can then be represented as follows:

$$U = \begin{pmatrix} \mathcal{I}_{3 \times 3} & & \\ & \mathcal{U}_{2 \times 2} & \\ & & \mathcal{I}_{3 \times 3} \end{pmatrix} . \quad (1)$$

Here  $\mathcal{I}$  are unit matrices. The subscripts indicate matrix dimensions while all the undisplayed elements are zero. The most general form of the matrix  $\mathcal{U}$  is

$$\mathcal{U} = \begin{pmatrix} 0 & e^{i\beta} \\ e^{i\alpha} & 0 \end{pmatrix} . \quad (2)$$

Our aim is to calculate the Hamiltonian  $H$  according to

$$U = e^{-iH\Delta t/\hbar} . \quad (3)$$

We adopt the usual approach in the quantum-computing literature [3.1-3.27] of assuming that the (constant) Hamiltonian  $H$  “acts” during the time interval  $\Delta t$ , i.e., we only consider evolution from  $t$  to  $t + \Delta t$ . The dynamics can be externally timed, with  $H$  being switched on at  $t$  and off at  $t + \Delta t$ . The time interval  $\Delta t$  is then related to the strength of couplings in  $H$  which are of order  $\hbar/\Delta t$ .

To obtain an expression for  $H$ , we calculate the “logarithm” of  $U$  in its diagonal representation. One can verify that the diagonalizing matrix  $T$ , such that  $T^\dagger U T$  is diagonal, is of the same structure as  $U$  in (1), with the nontrivial part  $\mathcal{U}$  replaced by  $\mathcal{T}$ , where

$$\mathcal{T} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta/2} & e^{i\beta/2} \\ e^{i\alpha/2} & -e^{i\alpha/2} \end{pmatrix} . \quad (4)$$

In the diagonal representation, the Hamiltonian is the diagonal  $8 \times 8$  matrix  $-\hbar A/\Delta t$ , where  $A$  has diagonal elements  $2\pi N_1, 2\pi N_2, 2\pi N_3, \frac{1}{2}(\alpha + \beta) + 2\pi N_4, \frac{1}{2}(\alpha + \beta) + \pi + 2\pi N_5, 2\pi N_6, 2\pi N_7, 2\pi N_8$ . Here  $N_j$  are arbitrary integers.

The Hamiltonian is then obtained as  $H = -\hbar T A T^\dagger / \Delta t$ , and it depends on the two (real) parameters  $\alpha$  and  $\beta$  and on the integers  $N_j$ . We restrict the number of parameters to obtain a specific example. In fact, we seek a Hamiltonian with few energy gaps [3.27]. However, we would also like to have a symmetric energy level structure. The following choice leads to a particularly elegant result for  $H$ . We put  $N_j = 0$  for  $j = 1, 2, 3, 6, 7, 8$ , and also  $\alpha + \beta + \pi + 2\pi(N_4 + N_5) = 0$  and  $N_5 - N_4 = N$ . This corresponds to the following energies:  $E_{1,2,3} = 0$ ,  $E_4 = \pi\hbar(N + \frac{1}{2})/\Delta t$ ,  $E_5 = -E_4$ ,  $E_{6,7,8} = 0$ .

The resulting Hamiltonian depends only on one real parameter,

$$\gamma = (\alpha - \beta)/2 , \quad (5)$$

and on one arbitrary integer,  $N$ . All the diagonal elements of the Hamiltonian will be zero with these choices of parameters. Indeed, calculation of  $H$  yields the result that this  $8 \times 8$  matrix with elements  $H_{mn}$ , where  $m$  labels the rows and  $n$  the columns, has only two nonzero entries,

$$H_{45} = \frac{\pi\hbar}{\Delta t} \left( N + \frac{1}{2} \right) e^{-i\gamma} \quad \text{and} \quad H_{54} = \frac{\pi\hbar}{\Delta t} \left( N + \frac{1}{2} \right) e^{i\gamma} . \quad (6)$$

Any matrix in a space with a multiple-qubit basis can be expanded in terms of the direct products of the four “basis”  $2 \times 2$  matrices for each of the two-level systems involved: the unit matrix  $\mathcal{I}$ , and the standard Pauli matrices  $\sigma_x, \sigma_y, \sigma_z$ . The latter are proportional to spin components for two-state systems which are the spin states of spin- $\frac{1}{2}$  particles. We will use the spin-component nomenclature, and their representation in terms of the Pauli matrices. We report here the result of such an expansion for the Hamiltonian  $H$ . While its matrix form is simple and only contains two nonzero elements, the spin-component representation is surprisingly complicated,

$$\begin{aligned} H = & \frac{\pi\hbar}{4\Delta t} \left( N + \frac{1}{2} \right) \\ & \times \left[ (\cos \gamma) (\sigma_x I \sigma_x C \sigma_x D - \sigma_x I \sigma_y C \sigma_y D + \sigma_y I \sigma_x C \sigma_y D + \sigma_y I \sigma_y C \sigma_x D) \right. \\ & \left. - (\sin \gamma) (\sigma_y I \sigma_y C \sigma_y D - \sigma_y I \sigma_x C \sigma_x D + \sigma_x I \sigma_y C \sigma_x D + \sigma_x I \sigma_x C \sigma_y D) \right] . \end{aligned} \quad (7)$$

### 3.3 Discussion

The fact that the Hamiltonian involves three-spin interactions suggests some interesting observations. The triplet  $x, y$ -component products are essential in the GHZ-paradox in quantum mechanics [3.41,3.42]. However, in that case these operators are *measured*. In fact, the need for multispin interactions in the Hamiltonian is a shortcoming as far as actual realizations, for instance, in the field of quantum computing, are concerned. Indeed, two-spin interactions are much more common and better understood theoretically and experimentally in solid-state and other systems, than three-spin interactions.

As mentioned earlier, our choice of the Hamiltonian is not unique. Its simplicity in the matrix form has allowed exact analytical result (7) be obtained. We have explored unitary transformation choices more general than (1). However, presently we cannot answer the question whether quantum signal splitting can be accomplished with two-spin interactions only.

The fact that “switching” is required, i.e., the interaction must be applied for a fixed duration of time, is also a difficulty, shared by all realistic proposals [3.1-3.27] for quantum-computing gates. Actually, time-variation of the form  $f(t)H$  is possible [3.27] during the time-interval  $\Delta t$ . Here the “protocol function”  $f(t)$  must average to 1 over the time interval:

$$(\Delta t)^{-1} \int_t^{t+\Delta t} f(t') dt' = 1 \quad , \quad (8)$$

and vanish outside the time-interval.

Finally, we comment that entanglement of one input spin in a general quantum state (not limited to the basis qubit states) with the states of two other spins has been utilized in quantum-computational error correction [3.13]. In that application, however, the two spins to be “mixed” with the input are initially in fixed states similar to the quantum copying procedures mentioned in the introduction.

In summary, we proposed a variant of the quantum copying/signal splitting in which the initial state is multiplied but there is uncertainty in which of the two-state systems involved is the multiple copy stored. The advantage of this scheme is that the initial copy-system states are not fixed. Explicit interaction Hamiltonian was derived for the three-spin case.

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## 4.0 Quantum Copying and the Controlled-NOT Gate

We derive an explicit Hamiltonian for copying the basis up and down states of a quantum two-state system—a qubit—onto  $n$  “copy” qubits ( $n \geq 1$ ) initially all prepared in the down state. In terms of spin components, for spin- $\frac{1}{2}$  particle spin states, the resulting Hamiltonian involves  $n$ - and  $(n + 1)$ -spin interactions. The case  $n = 1$  also corresponds to a quantum-computing controlled-NOT gate. (This section is self-contained.)

### 4.1 Introduction

Interest in quantum computing [4.1-4.27] has boosted studies of quantum mechanics of two-state systems such as the spin states of spin- $\frac{1}{2}$  particles. We will use “spin” to indicate a two-state system in this section. The “binary” up and down spin states are of particular significance and the two-state systems are also termed “qubits” in these studies. While macroscopic “desktop” coherent quantum computational units are still in the future [4.16,4.18], miniaturization of computer components calls for consideration of quantum-mechanical [4.14-4.16,4.18] aspects of their operation. Experiments have recently been reported [4.25,4.28-4.29] realizing the simplest quantum gates. Decoherence effects [4.16,4.18,4.26,4.30-4.32] and inherently quantum-mechanical computational algorithms [4.30-4.31,4.33-4.36] have been studied.

Here we consider the signal-copying process in two-state systems. We assume that  $n + 1$  spins are involved, where spin 1 is the input which is prepared in the up state,  $|1\rangle$ , or down state,  $|0\rangle$ , at time  $t$ . The aim is to obtain the same state in the  $n$  “copy” spin states, i.e., for spins  $2, 3, \dots, n + 1$ , as well as keep the original state of spin 1. Generally, one cannot copy an arbitrary [4.37-4.40] quantum state; however, one can duplicate a set of basis states such as the qubit states considered here. One can also discuss an approximate, optimized copying of the linear combinations of the basis states [4.39,4.40].

Another limitation of the copying procedure [4.37-4.40] has been that the *initial* state of the  $n$  copy spins must be *fixed*. An attempt to allow for a more general state leads to incomplete copying which is also of interest [4.41]. In this work we assume that the initial state, at time  $t$ , of all the copy spins is down,  $|0\rangle$ . Our aim is to derive an explicit Hamiltonian for the copying process.

We adopt the approach in the quantum-computing literature [4.1-4.27] of assuming that a constant Hamiltonian  $H$  acts during the time interval  $\Delta t$ , i.e., we only consider evolution from  $t$  to  $t + \Delta t$ . The dynamics can be externally timed, with  $H$  being switched on at  $t$  and off at  $t + \Delta t$ . The time interval is then related to the strength of couplings

in  $H$  which are of order  $\hbar/\Delta t$ . Some time dependence can be allowed [4.27], of the form  $f(t)H$ , where  $f(t)$  averages to 1 over  $\Delta t$  and vanishes outside this time interval.

We will denote the qubit states by quantum numbers  $q_j = 0$  (down) and  $q_j = 1$  (up), for spin  $j$ . The states of the  $n + 1$  spins will then be expanded in the basis  $|q_1 q_2 \cdots q_{n+1}\rangle$ . The actual copying process only imposes the two conditions

$$|100 \cdots 0\rangle \rightarrow |111 \cdots 1\rangle , \quad (1)$$

$$|000 \cdots 0\rangle \rightarrow |000 \cdots 0\rangle , \quad (2)$$

up to possible phase factors. Therefore, a unitary transformation that corresponds to quantum evolution over the time interval  $\Delta t$  is by no mean unique (and so the Hamiltonian is not unique). We will choose a particular transformation that allows analytical calculation and, for  $n = 1$ , yields a controlled-NOT Hamiltonian, as discussed later.

## 4.2 An Explicit Hamiltonian for Quantum Copying

We consider the following unitary transformation,

$$U = e^{i\beta} |111 \cdots 1\rangle \langle 100 \cdots 0| + e^{i\rho} |000 \cdots 0\rangle \langle 000 \cdots 0| \\ + e^{i\alpha} |100 \cdots 0\rangle \langle 111 \cdots 1| + \sum_{\{q_j\}'} |q_1 q_2 q_3 \cdots q_{n+1}\rangle \langle q_1 q_2 q_3 \cdots q_{n+1}| . \quad (3)$$

Here the first two terms accomplish the desired copying transformation. The third term is needed for unitarity (since the quantum evolution is reversible). We allowed for general phase factors in these terms. The sum in the fourth term,  $\{q_j\}'$ , is over *all the other* quantum states of the system, i.e., excluding the three states  $|111 \cdots 1\rangle$ ,  $|100 \cdots 0\rangle$ ,  $|000 \cdots 0\rangle$ . One could maintain analytical tractability while adding phase factors for each term in this sum; however, the added terms in the Hamiltonian are not interesting. One can check by explicit calculation that  $U$  is unitary,  $U^\dagger U = 1$ .

To calculate the Hamiltonian  $H$  according to

$$U = e^{-iH\Delta t/\hbar} , \quad (4)$$

we diagonalize  $U$ . The diagonalization is simple because we only have to work in the subspace of the three special states identified in (3), see the preceding paragraph. Furthermore, the part related to the state  $|000 \cdots 0\rangle$  is diagonal. In the subspace labeled



by  $|111 \cdots 1\rangle$ ,  $|100 \cdots 0\rangle$ ,  $|000 \cdots 0\rangle$ , in that order, the operator  $U$  is represented by the matrix

$$\mathcal{U} = \begin{pmatrix} 0 & e^{i\beta} & 0 \\ e^{i\alpha} & 0 & 0 \\ 0 & 0 & e^{i\rho} \end{pmatrix} . \quad (5)$$

The eigenvalues of  $\mathcal{U}$  are  $e^{i(\alpha+\beta)/2}$ ,  $-e^{i(\alpha+\beta)/2}$ ,  $e^{i\rho}$ . Therefore the eigenenergies of the Hamiltonian in the selected subspace can be of the form

$$E_1 = -\frac{\hbar}{2\Delta t}(\alpha + \beta) + \frac{2\pi\hbar}{\Delta t}N_1 , \quad (6)$$

$$E_2 = -\frac{\hbar}{2\Delta t}(\alpha + \beta) + \frac{2\pi\hbar}{\Delta t}\left(N_2 + \frac{1}{2}\right) , \quad (7)$$

$$E_3 = -\frac{\hbar}{\Delta t}\rho + \frac{2\pi\hbar}{\Delta t}N_3 , \quad (8)$$

where  $N_{1,2,3}$  are arbitrary integers.

In order to simplify the expressions, we will limit our consideration to a particular set of parameters. We would like to minimize energy gaps of the Hamiltonian [4.27] and generally, keep the energy spectrum symmetric. The latter condition yields a more elegant answer; actually, analytical calculation is possible with general parameter values. Thus, we take  $\rho = 0$ ,  $N_3 = 0$ , and also impose the condition  $E_1 + E_2 = 0$ . We then take the diagonal matrix with  $E_{1,2,3}$  as diagonal elements and apply the inverse of the unitary transformation that diagonalizes  $\mathcal{U}$ . All the calculations are straightforward and require no further explanation or presentation of details in the matrix notation. We note, however, that one could do all these calculations directly in the qubit-basis notation such as in (3); the diagonalization procedure is then the Bogoliubov transformation familiar from solid-state physics.

The result for the Hamiltonian in the three-state subspace is the matrix

$$\mathcal{H} = \frac{\pi\hbar}{\Delta t}\left(N - \frac{1}{2}\right) \begin{pmatrix} 0 & e^{-i\gamma} & 0 \\ e^{i\gamma} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} , \quad (9)$$

which depends on one real parameter

$$\gamma = \frac{\alpha + \beta}{2} \quad (10)$$

and on one arbitrary integer

$$N = N_1 - N_2 \quad (11)$$

The full Hamiltonian  $H$  in the  $2^{n+1}$ -dimensional spin space is

$$H = \frac{\pi\hbar}{\Delta t} \left( N - \frac{1}{2} \right) \left( e^{-i\gamma} |111 \dots 1\rangle \langle 100 \dots 0| + e^{i\gamma} |100 \dots 0\rangle \langle 111 \dots 1| \right) \quad (12)$$

In what follows we make the choice  $N = 1$  to simplify the notation. The form of the Hamiltonian is misleading in its simplicity. It actually involves  $n$ - and  $(n + 1)$ -spin interactions. To see this, we rewrite it in terms of direct products of the unit matrices and the standard Pauli matrices for spins  $1, \dots, n + 1$ , where the spins are indicated by superscripts (and  $N = 1$ ):

$$H = \frac{\pi\hbar}{2^{n+2}\Delta t} \left( 1 + \sigma_z^{(1)} \right) \left( e^{-i\gamma} \sigma_+^{(2)} \sigma_+^{(3)} \dots \sigma_+^{(n+1)} + e^{i\gamma} \sigma_-^{(2)} \sigma_-^{(3)} \dots \sigma_-^{(n+1)} \right) ; \quad (13)$$

here  $\sigma_{\pm} = \sigma_x \pm i\sigma_y$ ;  $\sigma_+ = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}$ ,  $\sigma_- = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}$ .

Multispin interactions are much less familiar and studied in solid-state and other systems than two-spin interactions. Therefore, the fact that for  $n = 1$  only single- and two-spin interactions are present is significant. In actual quantum-computing and other applications it may be more practical to make copies in stages, generating only one copy in each time interval, rather than produce  $n > 1$  copies simultaneously. Let us explore the  $n = 1$  case further. The Hamiltonian (with  $N = 1$ ) is, in terms of spin components (or rather the Pauli matrices to which the spin-component operators are proportional),

$$H_{n=1} = \frac{\pi\hbar}{4\Delta t} \left( 1 + \sigma_z^{(1)} \right) \left[ (\cos \gamma) \sigma_x^{(2)} + (\sin \gamma) \sigma_y^{(2)} \right] \quad (14)$$

This Hamiltonian involves two-spin couplings and also interactions which are linear in the  $x$  and  $y$  spin components. The latter may be due to a magnetic field applied in the  $xy$ -plane, at an angle  $\gamma$  with the  $x$  axis.

### 4.3 The Controlled-NOT Hamiltonian. Discussion

We note that the  $n = 1$  “single-copy” Hamiltonian also describes the controlled-NOT quantum gate with the same input and output spins. The truth table for the classical controlled-NOT can be written as follows in terms of the qubit states:

$$|11\rangle \rightarrow |10\rangle , \quad (15)$$

$$|10\rangle \rightarrow |11\rangle , \quad (16)$$

$$|01\rangle \rightarrow |01\rangle , \quad (17)$$

$$|00\rangle \rightarrow |00\rangle . \quad (18)$$

The “control” spin, 1, being up causes the other spin, 2, to flip. The control being down causes the second spin not to change.

The controlled-NOT unitary transformations have been discussed in the literature [4.7,4.13-4.15,4.28,4.42]. It is obvious that in the four-dimensional two-spin space labeled by  $|11\rangle, |10\rangle, |01\rangle, |00\rangle$ , in that order, the most general transformation matrix is of the form

$$U = \begin{pmatrix} 0 & e^{i\beta} & 0 & 0 \\ e^{i\alpha} & 0 & 0 & 0 \\ 0 & 0 & e^{i\omega} & 0 \\ 0 & 0 & 0 & e^{i\rho} \end{pmatrix} . \quad (19)$$

Our selected Hamiltonian accomplishes such a transformation (for  $n = 1$  only). The matrix  $U$  corresponding to (14) has the following choice of the phase factors,

$$U_{n=1} = \begin{pmatrix} 0 & -ie^{-i\gamma} & 0 & 0 \\ -ie^{i\gamma} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} . \quad (20)$$

Note that the details of this result depend on us setting  $N = 1$ .

In summary, we derived explicit Hamiltonians for  $n$ -copy quantum copying. For  $n = 1$ , the interactions are the most useful because they involve at most two-spin couplings. Furthermore, the  $n = 1$  Hamiltonian also corresponds to the controlled-NOT gate.

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## 5.0 SUMMARY

We initiated a research program to study the feasibility of quantum computing in condensed matter systems. The first step has been to consider the simplest quantum logic gates in order to identify which Hamiltonians are typical for interactions required for their operation. We have also identified future research directions and collaborations.

We studied the Hamiltonian for the quantum equivalent of the NOT computer gate. Explicit expression was obtained for the interaction parameters. Quantum signal splitting, of relevance to eavesdropping on transmission lines, has been investigated with emphasis on the way to accomplish a variant of signal splitting without limiting the initial quantum states of the systems in which the copies are recorded. Explicit interaction Hamiltonian was obtained. Quantum copying, important in error-correction protocols, has been investigated with the aim of deriving an explicit Hamiltonian for the process.

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